Contribution ID: **32** Type: **Poster Presentations**

Halogen and non-metals defects induced n- and p-type conductivity in monolayer MoS2 two-dimensional semiconductor

Friday, 20 November 2020 17:25 (1 hour)

Recent developments from the doping of two-dimensional (2D) monolayer MoS2 has opened up the possibility of scaling down the thickness of semiconductors channel field-effect transistors to the sub-nanometer scale. In order to realise efficient MoS2 based devices including p-n junction and field-effect-transistor for optimal performance, a controlled doping system needs to be fully understood.

In this report, a systematic effective method of doping in order to realise a p- or n-type conductivity in monolayer MoS2 was predicted using density functional theory with the aid of the generalised gradient approximation. The structural, electronic and magnetic properties of halogens and group V atoms substitution, interstitial and vacancy-complexes of monolayer MoS2 were investigated. While the substitutional and vacancy complexes are more energetically favourable under the Mo-rich chemical potential conditions, the interstitial do not have preference for any chemical potential limit conditions. The substitutional defects are more energetically favourable than the interstitial in both the Mo-rich and S-rich chemical potential conditions. Whereas the group V substitutional defects are good candidate for p-type conductivity, the halogen substitutions are good candidate for n-type conductivity. The substitution of the group V and halogen atoms induced spin polarisation in the host with a total magnetic moment of 1.00 μB. The defect complexes are stable with respect to their binding energies. While the vacancy-complexes formed by VS and NS, PS, AsS behave as p-type semiconductors, those formed by the SbS and BiS exhibit metallic characters.

In addition to providing useful hint for device fabrication where spin polarisation are required, the results presented here could paved the way for more insight to realising enhanced p and n-type conductivity of defective monolayer MoS2 2D semiconductor

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Track Classification: AfLS2020 track